

# The Problem of Ground State in Thermo-Field Dynamics.

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## Abstract

Analytic continuation of quantum statistical physics from imaginary to real time is analyzed. Adiabatic vanishing of interactions at real time infinities gives origin to singularities at complex times. This undermines the hypothesis of decoupling of interactions at  $t \rightarrow \infty$ . Hence an interacting thermal vacuum is a necessary component of the exact real-time formalism. Consequences for TFD are discussed.

## 1 Introduction

Usually quantum statistical physics is formulated in terms of density matrix (DM). In equilibrium it is given by Gibbs formula [1]

$$\rho = \sum_{n=0}^{\infty} |n\rangle \exp -\beta E_n \langle n|, \quad (1)$$

$\beta$  being inverse temperature and  $E_n$  standing for the energy of the  $n$ -th level. The trace of  $\rho$  defines thermodynamic functions and kinetic properties are governed by the evolution of DM [2].

The idea of thermo-field dynamics (TFD) is to consider instead a quantum field theory formulated in a special thermal vacuum (TV) [3, 4]  $|O(\beta)\rangle$ . Expectation values should coincide with the averages calculated by means of DM.

$$\hat{A} = \langle O(\beta) | \hat{A} | O(\beta) \rangle = \text{tr } \rho \hat{A}. \quad (2)$$

Kinetic properties are defined by time dependent correlation functions in TV.

$$\langle \hat{A}(t) \hat{B}(0) \rangle = \langle O(\beta) | \hat{A} \exp(-i\hat{H}t) \hat{B} | O(\beta) \rangle. \quad (3)$$

It's well known that the number of degrees of freedom is doubled in TFD: every physical field  $\phi$  enters with the corresponding "ghost"  $\tilde{\phi}$ . Physical density matrix is obtained after the convolution of  $|O(\beta)\rangle \langle O(\beta)|$  with respect to the tilde-fields.

$$\rho = \tilde{\text{tr}} |O(\beta)\rangle \langle O(\beta)| \quad (4)$$

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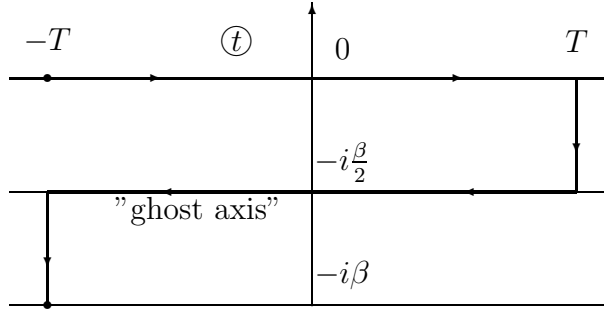


Figure 1: The contour  $C_{TFD}$  used to derive real-time formalism. Physical fields live on the real time axis and tilde-fields are defined on the "ghost axis"  $\text{Im } t = -\beta/2$ .

The obvious advantage is that TFD looks like the ordinary field theory. Real time formalism (RTF) immediately extends the scope to kinetic problems. The less transparent benefit is cancellation of higher powers of  $\delta$ -functions [5, 4]. Those appear when one takes into account beads of self-energy corrections to propagators of real particles in the heat bath. Fortunately the contribution of ghosts cancels poorly defined terms.

The structure of TFD and the origin of ghosts are much more transparent in the time-path (TP) method [5]. It claims that TFD and familiar Matsubara technique are linked by an analytic continuation. The subject of the talk are problems met by this method in interacting theories. The procedure looks safe at the level of free fields. However in presence of perturbations there are singularities in complex time plane restricting deformations of TP [6]. Physically this reflects the difference between interacting and noninteracting thermal vacua.

## 2 Time-Path Method

We shall sketch the analytic continuation relating TFD to Matsubara imaginary-time formalism [5, 4]. The free energy of a quantum system is

$$F = -\frac{1}{\beta} \log \text{tr} \exp -\beta \hat{H} \quad (5)$$

In Matsubara approach it is treated as a quantum field generating functional [7, 8] for the evolution during finite imaginary time  $-i\beta$ . Bose-fields are  $\beta$  periodic and Fermi-fields are antiperiodic in this coordinate. The time interval of evolution is portrayed by the contour  $C^M$  in complex time plane (see Fig. 2.).

It proves that  $F$  is invariant with respect to deformations preserving monotonous decrease of  $\text{Im } t$  along the contour [9]. Consider the deformation shown in Fig. 1. It turns out that in the limit  $T \rightarrow \infty$  for free fields one obtains the formulae of TFD. Physical fields are defined on the real time axis and "tilde"-fields live on the "ghost axis"  $\text{Im } t = -\beta/2$ .

The usual assumption is that the vertical pieces decouple as  $T \rightarrow \infty$ . That infers that they result only into a multiplicative renormalization of the statistical sum and do not contribute significantly to thermodynamic functions.

### 3 Adiabatic perturbations and complex time singularities

Usually one implies in QFT that interaction is absent at  $t = \pm\infty$  and turns on adiabatically in physical domain. Thus asymptotic states are free. They form a complete set used as a basis in calculations.

Decoupling of vertical sections of the TFD-path also suggests that the asymptotic states are the same as without perturbation. So the latter might be turned off adiabatically at real time infinities. However in thermal theories these adiabatic changes give rise to singularities of the perturbation at complex times [6]. The latter restrict deformation of the time-path making noninteracting area inaccessible. This indicates that interaction modifies the ground state and thermal vacuum may differ substantially from the set of free thermal quanta.

To prove the existence of singularities let's recall the general properties of perturbation. It's natural to believe that:

- (a) Perturbation  $V$  is real on the real time axis and because of analyticity  $V(\bar{t}) = \bar{V}(t)$ . (Bar stands for complex conjugation.)
- (b) In physical region  $V(|t| \ll T) \approx \text{const}$  and  $V(t = \pm\infty) = 0$ .
- (c) Perturbation  $V(t)$  is periodic in imaginary time with the period  $i\beta$ .

The last requirement means that  $V(t)$  has the same temperature as the nonperturbed system. Otherwise we encounter a nonequilibrium situation and heating processes occur.

The TPM is applicable if  $V(t)$  is analytic throughout the strip  $-\beta < \text{Im } t < 0$ . Meanwhile the requirements (b) and (c) are fulfilled simultaneously only for functions with singularities in this region. One can prove this in the following way.

- (i) Periodicity makes the domain of definition of  $V$  topologically equivalent to an infinite cylinder.
- (ii) The condition (b) permits to add points  $t = \pm\infty$  converting the cylinder to a sphere.
- (iii) The number of zeros of a function analytic on a sphere is equal to that of poles. Hence  $V$  has in the strip **at least two simple poles**. (The case of a second order pole contradicts  $V \approx \text{const}$  in physical region.)<sup>1</sup>

Hereon we shall discuss this simplest case.

It is easy to show that the singularities are symmetric with respect to the ghost axis  $\text{Im } t = -\beta/2$ .

- (i) According to (a) there should be a pole 2 at  $\text{Im } t = \frac{\beta}{2} + \Delta$  if there is a pole 1 at  $\text{Im } t = -\frac{\beta}{2} - \Delta$ .
- (ii) Periodicity immediately requires the existence of a pole 3 at  $\text{Im } t = -\frac{\beta}{2} + \Delta$ .
- (iii) The poles 1 and 3 are symmetric with respect to the ghost axis.

Proceeding in an analogous way one can prove that  $V(t)$  must be real on the ghost axis.

We can find residues of  $V$  at the poles (or the integral over the border of the analytic domain for more elaborate singularities, Fig.4). To do that we shall integrate  $V$  along the contours  $C_1$ ,  $C_2$  shown in Fig.2. The integral can be split into a sum of the four pieces.

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<sup>1</sup>I shall call these poles Hoo-Doos after the ghosts watching the horizons of Banff on foggy days.

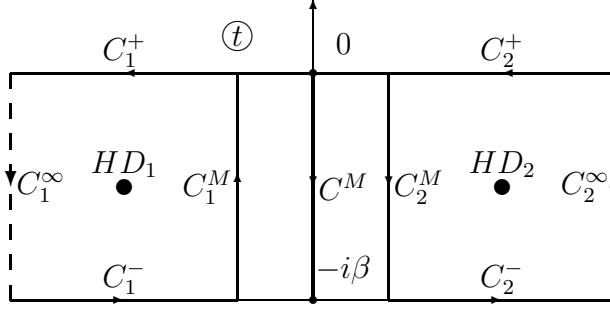


Figure 2: Matsubara contour  $C^M$  and contours  $C_{1,2}$  used to calculate the residues at the poles  $HD_{1,2}$ .

$$\oint_C = \int_{C^M} + \int_{C^-} + \int_{C^+} + \int_{C^\infty} \quad (6)$$

The last is zero because of (b) and periodicity is a reason for cancellation of the 2-nd with the 3-rd. Thus

$$\text{res}_{1(2)} V(t) = (-) \frac{1}{2\pi i} \int_{C_M} V(t) dt = (-) \left( -\frac{\beta V}{2\pi} \right) \quad (7)$$

The result is absolutely natural. (Note that the nonzero residues are an independent proof of the existence of singularities.)

Finally let us give an example of a function possessing all the listed properties (a)–(c).

$$V(t) = V_0 \frac{1 + \cosh \frac{2\pi t_{HD}}{\beta}}{\cosh \frac{2\pi t}{\beta} + \cosh \frac{2\pi t_{HD}}{\beta}} \quad (8)$$

It is  $i\beta$  periodic and has poles at the points  $\pm t_{HD} + i\beta(n - \frac{1}{2})$ . It vanishes at real time infinities and  $V(|t| \ll t_{HD}) \approx V_0$ . The residues are  $\frac{\beta}{2\pi} V(0) + O(e^{-\frac{4\pi t_{HD}}{\beta}})$ .

## 4 The problem of interacting thermal vacuum

The complex time singularities restrict deformations of time paths, Fig.3.

In fact this evidences that thermal theories are selfconsistent only if the vacuum state is interacting. As long as the vertical sections of the RTF-contour lay in the physical domain where  $V \neq 0$  one deals indeed with an analytic continuation of the imaginary time Matsubara approach. However neglecting the contribution of the vertical pieces is not an analytic procedure.

Strictly speaking that means that interacting TFD is not an analytic continuation of imaginary time methods. A question arises what are the cases when this beautiful theory gives good approximations and when the discrepancy with conservative approaches becomes essential.

The complete analytic continuation begins with the solution of quantum statistical (Matsubara) problem. The difference comes forth from the dependence of thermal vacuum on



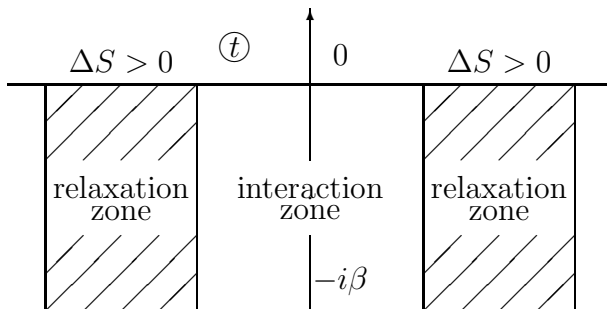


Figure 4: In realistic systems analyticity is broken by relaxation processes.

## 5 Discussion and examples

Now we shall briefly discuss some cases where sensitivity to the interaction in the initial state can be important. Somehow all listed here happen to deal with some aspects of the ground state symmetry.

The first example are theories with spontaneously broken symmetry (*e.g.*  $\lambda\varphi^4$ -theories). It is well known that quantum corrections make effective potential temperature dependent [10]. At high temperatures symmetry restoration takes place. Thus the ground state (*i.e.* thermal vacuum) depends both on temperature and interaction. The naive approach is unsuitable in this case.

Interaction can form new states in the energy spectrum. (The arising difficulties are not specific to TFD alone.) If it is the case the noninteracting basis is incomplete and the theory can not be formulated in terms of the free fields. The classic example is that of superconductivity where the existence of condensate is an assumption necessary for a successful treatment.

New states with high energy are not so important and the most prominent contributions come from zero modes, *i.e.* states  $|\psi_0\rangle$  with zero energy:  $(\hat{H} + \hat{V})|\psi_0\rangle = 0$ . These states violate conditions of Riemann-Lebesgue lemma which is crucial in the proof of decoupling [4].

The more general are cases of so called quantum algebras [11]. (These should be not mixed with those studied in connection with string and conformal field theories.) Here the interacting thermal vacuum belongs to nontrivial representation of the corresponding group whereas the free one by definition is a singlet. The transformation properties impose selection rules on expectation values. This sort of situation was found to take place in Anderson model [12] where  $|O(\beta)\rangle = \otimes_i |O(\beta)\rangle_i$  and operators from different sectors enter calculations accompanied by different sets of closed vacuum graphs.

Finally we shall discuss a simple case where the assumption about initial state immediately affects the calculation. Imagine a system of noninteracting  $\frac{1}{2}$ -spins in a magnetic field  $h$  which is treated as a perturbation. (This generalizes to arbitrary degenerate levels which are split by some interaction.) It happens that pure quantum mechanical evolution which begins from noninteracting (*i.e.* degenerate) state is unable to provide a nonzero magnetization in this system.

The hamiltonian  $\hat{H}$  and the perturbation  $\hat{V}$  are

$$\hat{H}_0 = 0; \quad \hat{V}_0 = -\frac{1}{2}\sigma_z h; \quad (13)$$

The degenerate *in*-state is written as follows (we shall proceed using both TFD and DM formalisms).

$$|O(\beta, 0)\rangle = \frac{1}{\sqrt{2}}[|\uparrow\tilde{\uparrow}\rangle + |\downarrow\tilde{\downarrow}\rangle]; \quad \rho(0) = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (14)$$

Their evolutions are governed by the full hamiltonians

$$\hat{H}_{TFD} = \hat{V} - \hat{\tilde{V}}; \quad \hat{H}_{DM} = \hat{V}. \quad (15)$$

The laws of evolution are:

$$|O(\beta, t)\rangle = \exp(-i\hat{H}_{TFD}t)|O(\beta, 0)\rangle; \quad \rho(t) = \exp(-i\hat{H}_{DM}t)\rho(0)\exp(i\hat{H}_{DM}t) \quad (16)$$

Without much effort one sees that  $|O(\beta, t)\rangle$  and  $\rho(t)$  do not change and the states remain degenerate despite the interaction. Hence there is no magnetization in this approach which certainly is wrong.

Meanwhile taking the perturbation into account from the very beginning gives:

$$|O(\beta)\rangle_V = \frac{|e^{\frac{\beta h}{4}}\uparrow\tilde{\uparrow}\rangle + e^{-\frac{\beta h}{4}}|\downarrow\tilde{\downarrow}\rangle}{\sqrt{2}\cosh\frac{\beta h}{2}}; \quad \rho_V = \frac{1}{2\cosh\frac{\beta h}{2}} \begin{pmatrix} e^{\frac{\beta h}{2}} & 0 \\ 0 & e^{-\frac{\beta h}{2}} \end{pmatrix} \quad (17)$$

Which leads to the known value

$$M_z = \frac{1}{2} \tanh \frac{\beta h}{2} \quad (18)$$

The example demonstrates that some physical quantities are especially sensitive to particular details of the structure of thermal vacuum. In our case magnetization was the one feeling the degeneracy of states. Quantum mechanics disregards relaxation and systems have a memory of the initial state. This is not the case for statistical physics. Generally some special improvements of thermal vacuum should be made by hand in order to obtain the correct values of sensitive quantities.

## 6 Summary

We have shown that adiabatically changing perturbations can not be safely incorporated in thermal theory framework. For interacting theory the real time formalism has been shown not to be an analytic continuation of the imaginary time technique. That means that TFD is not a new guise of the Matsubara approach. The use of noninteracting thermal vacuum is an approximation which needs justification in particular cases. The reason for that is not simply striving for mathematical rigorousness but sensitivity of certain physical quantities to the details of the structure of the ground state.

The tool for analyzing a thermal vacuum is the interacting imaginary time formalism. With the help of it one can find out if the nonperturbed TFD vacuum is good enough for a specific problem and decide what should be the necessary *a priori* improvements. With the corrected vacuum state all the power and beauty of TFD are welcome and the circumspect ones may no longer be afraid of Hoo-Doos on the chosen trail.

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